

PT-symmetric quantum models living in an auxiliary Pontryagin space

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Abstract

The recent heuristic as well as phenomenological success of the use of non-Hermitian Hamiltonians which are required self-adjoint in a Krein space \mathbf{K} is recalled, and an extension of the scope of such a version of quantum theory is proposed. The usual choice of the indefinite metric \mathcal{P} treated as the operator of parity is generalized. *In nuce*, the operators \mathcal{P} are admitted to represent the indefinite metric in a Pontryagin space $\tilde{\mathbf{K}}$. A constructive version of such a generalized quantization strategy is outlined and found feasible.

1 Introduction

In the most common applications of quantum theory [1] the norm-preserving time-evolution of a non-relativistic quantum system is controlled by a self-adjoint Hamiltonian $\hat{H} = \hat{H}^\dagger$. One starts from its form defined, typically, as a sum of kinetic energy $-\Delta$ and of an interaction-energy potential $V(x)$. The resulting operator is assumed acting in a friendly Hilbert space $\mathbf{H}^{(F)}$ represented, say, by the linear space $L^2(\mathbb{R})$ of quadratically integrable functions. In the Schrödinger's mode of description the states are ket vectors $|\psi(t)\rangle$

living in $\mathbf{H}^{(F)}$. Their form may be determined via Schrödinger equation

$$i\partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle, \quad |\psi(t)\rangle \in \mathbf{H}^{(F)}. \quad (1)$$

In constructive considerations, unitary Fourier-like transformations Ω of $\mathbf{H}^{(F)}$ are often used leading to the strictly equivalent physical predictions. Once the Fourier-like maps Ω are allowed more general and non-unitary, the images $\Omega |\psi(t)\rangle^{(F)} := |\psi(t)\rangle^{(P)}$ of the kets $|\psi(t)\rangle^{(F)} \in \mathbf{H}^{(F)}$ should be treated as transferred into a *non-equivalent* Hilbert space, $|\psi(t)\rangle^{(P)} \in \mathbf{H}^{(P)}$ [2].

Whenever the “friendly” space $\mathbf{H}^{(F)}$ is assumed unphysical, we are well motivated to treat the other space $\mathbf{H}^{(P)}$ as correct and “physical”. If the new space $\mathbf{H}^{(P)}$ remains friendly, we may just change the Hamiltonian operator accordingly,

$$\Omega : H \rightarrow \mathfrak{h} := \Omega H \Omega^{-1}. \quad (2)$$

The truly nontrivial situation only emerges when the new, self-adjoint Hamiltonian \mathfrak{h} defined in $\mathbf{H}^{(P)}$ becomes prohibitively complicated. Then, the pull-back of the Hermiticity condition to the friendly space is still recommendable yielding the hidden Hermiticity rule (a.k.a. “crypto-Hermiticity” or “quasi-Hermiticity”)

$$H^\dagger \Theta = \Theta H, \quad \Theta = \Omega^\dagger \Omega \quad (3)$$

postulated directly in the friendly space $\mathbf{H}^{(F)}$ and, historically, attributable to Dieudonné [3].

In the present paper we intend to pay attention to the details of the path between the “false” initial Hilbert space $\mathbf{H}^{(F)}$ and its concrete, correct and “physical” amendment $\mathbf{H}^{(P)}$. We shall analyze and generalize one of the most popular strategies of transition $\mathbf{H}^{(F)} \rightarrow \mathbf{H}^{(P)}$ which makes a detour via an intermediate auxiliary Krein space \mathbf{K} (based on the use of an indefinite (pseudo)metric \mathcal{P}) and which might be called \mathcal{PT} –symmetric quantum mechanics (PTSQM, [4] – more comments and explanations will be added below).

2 The quantization recipe based on the \mathcal{PT} symmetry

Our interest in the possibility of an amendment of the PTSQM recipe was inspired by the particular success of the removal of the ambiguity of $\Theta_\alpha(H)$ based on the *ad hoc* PTSQM assumption that at $\alpha = \alpha_{\text{exceptional}}$, the product $\mathcal{P}\Theta_\alpha(H)$ might preserve certain mathematical properties of the parity [5] or, alternatively, that it could acquire certain phenomenological features of the charge [6].

In both of the latter scenarios, the most natural mathematical interpretation of the operator \mathcal{P} may be seen in its role of a Krein-space (pseudo)metric. On such a background, the core of our present main proposal will lie in the replacement of the intermediate Krein space \mathbf{K} by the alternative intermediate Pontryagin space $\tilde{\mathbf{K}}$, dictated by the intention of making the auxiliary

pseudometric operator \mathcal{P} much less dependent upon the phenomenological notion of the observable parity.

Our present second guiding idea is that due to the isospectrality of H , H^\dagger and \mathfrak{h} one often finds it useful to stay working inside $\mathbf{H}^{(F)}$. A persuasive illustration of such a three-Hamiltonian strategy and scenario has been offered, almost twenty years ago, by nuclear physicists [7]. Nevertheless, from the purely practical and heuristic point of view, the ultimate and decisive amendment of the recipe only appeared in the context of field theory [8, 9]. The most productive trick has been found in an *additional* postulate

$$H^\dagger \mathcal{P} = \mathcal{P} H. \quad (4)$$

The latter property of the Hamiltonian (where the symbol \mathcal{P} denotes, most often, the operator of parity) is called its \mathcal{PT} -symmetry (cf., e.g., reviews [4, 10] for an explanation of this terminological convention).

We should emphasize that in the major part of the recent literature on \mathcal{PT} -symmetry in physics the phenomenological Hamiltonian is assumed given as a non-self-adjoint operator $\hat{H} \neq \hat{H}^\dagger$ acting in an unphysical Hilbert space $\mathbf{H}^{(F)}$ and exhibiting the additional “symmetry” (4). As long as the underlying class of the admissible non-unitary Hermitization mappings Ω is only very weakly restricted in such a case, one of the main weak points of the theory may be seen in the ambiguity of the assignment $H \rightarrow \mathfrak{h}$ given by Eq. (2), i.e., in the ambiguity of the choice of the “metric” operator out of a family $\Theta = \Theta_\alpha(H)$ where $\alpha = 1, 2, \dots$ [7].

The assumption of simplicity of the (pseudo)metrics \mathcal{P} and the additional natural assumption of its involutivity $\mathcal{P}^2 = I$ usually decisively facilitate the construction of the physical Hilbert space $\mathbf{H}^{(P)}$. In some considerations, it makes sense to treat the Hilbert space $\mathbf{H}^{(P)}$ as a single element of the whole family of the mutually unitarily equivalent spaces among which a “special” one will be denoted by the symbol $\mathbf{H}^{(S)}$ – according to Ref. [2] its superscript $^{(S)}$ might mean a “synthesis” or “sophistication”.

In our compact review paper [2] we proposed that the relation between the equivalent representations $\mathbf{H}^{(P)}$ and $\mathbf{H}^{(S)}$ of the physical Hilbert space of states might be visualized as an equivalence in which one works with the respective generalized inner products $\langle \psi | \phi \rangle \rightarrow \langle \psi | \phi \rangle^{(P,S)} := \langle \psi | \Theta^{(P,S)} | \phi \rangle$ using the concept of the *ad hoc* metric operators such that $\Theta^{(S)} \neq \Theta^{(P)} \equiv I$. In other words, one can speak about a metric-dependent definition of the conjugation in $\mathbf{H}^{(S)}$. In this manner one updates the usual, “friendly” (sometimes called “Dirac’s”) Hermitian conjugation of vectors,

$$\mathbf{T}^{(F)} : |\psi(t)\rangle \rightarrow \langle \psi(t)| \quad (5)$$

which is active in the auxiliary, unphysical Hilbert space $\mathbf{H}^{(F)}$. In the update one replaces it by the metric-dependent prescription

$$\mathbf{T}^{(S)} : |\psi(t)\rangle \rightarrow \langle\langle \psi(t) | := \langle \psi(t) | \Theta. \quad (6)$$

The latter recipe should be read as active in the sophisticated physical Hilbert space $\mathbf{H}^{(S)}$, the kets of which coincide with those of $\mathbf{H}^{(F)}$. For our present

purposes the prescription (6) may be identified, therefore, with the traditional Hermitian conjugation used in the unusual, “sophisticated” space $\mathbf{H}^{(S)}$.

The mathematics which is hidden behind the transition from Eq. (5) to Eq. (6) is fairly nontrivial. For this reason (and also for the sake of brevity of our forthcoming considerations) let us circumvent, in the present paper, the majority of the technical subtleties connected with the underlying functional analysis and let us restrict our attention just to the finite-dimensional vector-space versions of the triplet of the Hilbert spaces $\mathbf{H}^{(F,S,P)}$ in question.

3 Illustrative Jacobi-matrix toy-model Hamiltonians

As we already mentioned, one of the most important emerging questions (formulated and answered, in the context of physics, by Scholtz et al [7]) concerns the ambiguity and/or possibility of an identification of an “optimal” Hilbert space $\mathbf{H}^{(S)}$ for a given Hamiltonian \hat{H} with the real spectrum. In the brief summary of this point let us employ the notation of review [2] where we suggested to write the “hidden” Hermiticity condition in $\mathbf{H}^{(S)}$ in the following abbreviated form

$$\hat{H} = \hat{H}^\ddagger := \Theta^{-1} \hat{H}^\dagger \Theta. \quad (7)$$

The superscript † stands here for the “Dirac’s” transposition plus complex conjugation as defined by Eq. (5) for vectors and as used, in the $N \rightarrow \infty$ limit, in the most common auxiliary-space representations $\mathbf{H}^{(F)} = \ell^2(\mathbb{Z})$ or $\mathbf{H}^{(F)} = \mathbb{L}^2(\mathbb{R})$ with $\Theta^{(F)} \equiv I$. In this notation the “doubled superscript” ‡ marks the (crypto)hermitian conjugation of Eq. (7) for the operators in $\mathbf{H}^{(S)}$. In this manner the cryptohermitian conjugation (6) of vectors is extended to the cryptohermitian conjugation of operators in $\mathbf{H}^{(S)}$. Both these relations contain the same nontrivial metric operator $\Omega^\dagger \Omega = \Theta = \Theta^{(S)} \neq I$.

3.1 Multiparametric chain models exhibiting an up-down symmetry

In the physics literature as reviewed briefly in Ref. [11] we witness an intensification of interest in the real and N –dimensional tridiagonal-matrix Hamiltonians. The main reason is that these Hamiltonians $\hat{H}^{(N)}$ describe a rather universal N –site quantum-lattice dynamics in which just the nearest-neighbor interaction is taken into account. The second reason is that these models are nontrivial in the sense that the real matrix $\hat{H}^{(N)}$ itself (possessing, presumably, real and non-degenerate spectrum) may remain asymmetric, i.e., manifestly non-Hermitian in the linear-algebraic sense, $\hat{H}^{(N)} \neq \left[\hat{H}^{(N)} \right]^\dagger$.

In the language of physics the role of the latter Hamiltonians (which cannot generate the unitary evolution inside the most common real vector space $\mathbf{H}^{(F)}$) may be seen in their intimate connection with experiments [12]. At the same time their mathematical analysis may significantly be simplified

via a specific choice of the matrix elements in $\hat{H}^{(N)}$. In Refs. [13], for example, we assumed that Hamiltonian $\hat{H}^{(N)}$ representing a finite-dimensional anharmonic-oscillator-like model is a diagonal matrix (with an equidistant unperturbed spectrum) which is complemented by a small antisymmetric term mimicking the nearest-neighbor interaction of a chain-model type.

We revealed that an enormous simplification of the analysis appears when one adds another requirement of a parity-type symmetry of the (real) matrix with respect to its second diagonal,

$$H^{(chain)} = \begin{bmatrix} 1-N & g_1 & 0 & 0 & \dots & 0 \\ -g_1 & 3-N & g_2 & 0 & \dots & 0 \\ 0 & -g_2 & 5-N & \ddots & \ddots & \vdots \\ 0 & 0 & \ddots & \ddots & g_2 & 0 \\ \vdots & \vdots & \ddots & -g_2 & N-3 & g_1 \\ 0 & 0 & \dots & 0 & -g_1 & N-1 \end{bmatrix} \neq (H^{(chain)})^\dagger. \quad (8)$$

In spite of the presence of many independent coupling constants such a symmetry proved sufficient to guarantee the reality of the spectrum even far beyond the weak-coupling dynamical regime. Thus, the “hidden” Hermiticity materializes via the transition to the “second physical” Hilbert space $\mathbf{H}^{(S)}$ in a fairly large and non-numerically defined cryptohermiticity domain $D = D(g_1, g_2, \dots, g_J)$ of as many as $J = \text{entier}[N/2]$ independently variable couplings.

The pragmatic appeal of multiparametric models (8) has been weakened by the purely numerical nature of the eligible metrics $\Theta^{(N)}$ defining the alternative Hilbert spaces $\mathbf{H}^{(S)}$. In the subsequent, more constructive studies [14, 15] and [16] we diminished our phenomenological ambitions, therefore. We turned attention to the more elementary, square-well-type discrete Hamiltonian matrices endowed with the mere one-parametric point-like Hermiticity-violating interaction terms located either near the center or near the boundary walls, respectively. For example, the option of Ref. [16] with

$$H^{(N)}(\lambda) = \begin{bmatrix} 2 & -1-\lambda & 0 & \dots & 0 & 0 \\ -1+\lambda & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & -1 & 0 \\ 0 & \vdots & \ddots & -1 & 2 & -1-\lambda \\ 0 & 0 & \dots & 0 & -1+\lambda & 2 \end{bmatrix} \quad (9)$$

enabled us to reach a certain next-to-solvable status of transparency of transitions between the unphysical and physical Hilbert spaces $\mathbf{H}^{(F)}$ and $\mathbf{H}^{(S)}$, respectively. For the latter family of non-unique candidates for the physics-representing Hilbert spaces we were able to offer a manifestly constructive and *complete* classification of the admissible metrics $\Theta = \Theta(H)$.

3.2 Asymmetric solvable models

A residual weakness of the latter model (9) has been felt in a comparatively complicated structure of its bound-state eigenvectors. This observation motivated our subsequent search for another one-parametric toy-model Hamiltonian characterized by a non-numerical solvability of Schrödinger equation

$$\hat{H}^{(N)} |\psi_n\rangle = E_n |\psi_n\rangle, \quad n = 0, 1, \dots, N-1 \quad (10)$$

in $\mathbf{H}^{(F)}$ at any matrix dimension $N = 1, 2, \dots$. A very special Hamiltonian of the required type, viz.,

$$\hat{H}^{(N)} := H^{(N)}(a) = \begin{bmatrix} a+1 & -1 & 0 & 0 & \dots \\ -a-1 & a+3 & -2 & 0 & \dots \\ 0 & -a-2 & a+5 & -3 & \ddots \\ 0 & 0 & -a-3 & a+7 & \ddots \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{bmatrix} \quad (11)$$

has been proposed in Ref. [11]. Such a Hamiltonian must be truncated. At finite cut-offs $N < \infty$ it offers an interesting phenomenological model admitting the non-numerical diagonalization as well as a systematic construction of the complete set of the eligible metrics Θ via Dieudonné equation. Unfortunately, the loss of the up-down symmetry in model (11) proved to lead to a loss of the nice properties in the limit $N \rightarrow \infty$. For this reason we finally decided to turn our attention to a compromising asymmetric version of model (9) here,

$$H^{(N)}(\lambda) = \begin{bmatrix} 2 & -1-\lambda & 0 & \dots & 0 & 0 \\ -1+\lambda & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & \ddots & \ddots & \vdots \\ \vdots & 0 & \ddots & \ddots & -1 & 0 \\ 0 & \vdots & \ddots & -1 & 2 & -1+\lambda \\ 0 & 0 & \dots & 0 & -1-\lambda & 2 \end{bmatrix}. \quad (12)$$

For this model we revealed, in Ref. [15], that the simplifying role of the up-down symmetry need not be decisive. In particular, although the necessary solutions E_n and $|\psi_n\rangle$ of the underlying time-independent Schrödinger's bound-state problem (10) remained numerical, we were able to avoid the necessity of their construction (needed, first of all, in the spectral formula for the metrics) by the non-numerical construction of the metrics via the computer-assisted direct solution of the Dieudonné's equation. In this sense our present text may be read as a continuation and as a climax of the study initiated in Ref. [15].

4 The energies and metrics

4.1 The reality of the spectra of $H^{(N)}(\lambda)$.

At any $N = 3, 4, \dots$ and $\lambda \in (-1, 1)$ let us consider the finite-dimensional-matrix N by N toy Hamiltonians $H^{(N)}(\lambda)$ of Eq. (12). They will be shown suitable for illustration of our present reinterpretation of Eq. (4). First of all, the spectrum of their energies is very easily evaluated at $N = 3$,

$$E_0 = 2, \quad E_{\pm 1} = 2 \pm (2 - 2\lambda^2)^{1/2}$$

as well as at $N = 4$,

$$E_{\pm 1/2} = 3/2 \pm 1/2(5 - 4\lambda^2)^{1/2}, \quad E_{\pm 3/2} = 5/2 \pm 1/2(5 - 4\lambda^2)^{1/2}$$

(cf. Fig. 1) or at $N = 5$,

$$E_0 = 2, \quad E_{\pm 1} = 2 \pm (1 - \lambda^2)^{1/2}, \quad E_{\pm 2} = 2 \pm (3 - \lambda^2)^{1/2}$$

etc. One always encounters precisely four fragile levels which intersect at $\lambda = \pm 1$ at even N and which do not intersect at odd N . A clear distinction emerges between the even and odd dimensions N : one always finds a λ -independent central level $E_0 = 2$ in the latter case (cf. the $N = 7$ illustrative example in Fig. 2). Inside the interval of $\lambda \in (-1, 1)$ the spectrum is discrete, up-down symmetric, non-degenerate and real at any N (cf. the proof in [15]).

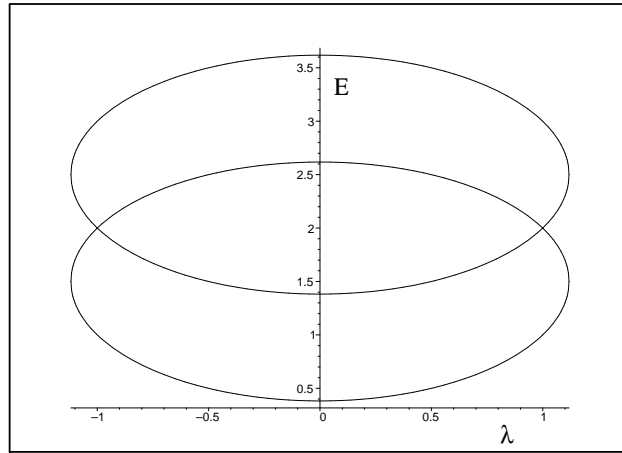


Figure 1: Graphical form of spectrum at $N = 4$.

4.2 Dieudonné equation and its definite/indefinite solutions.

Equation (4) may be treated as a linear algebraic constraint

$$\sum_{k=1}^N \left[(H^\dagger)_{jk} \Theta_{kn} - \Theta_{jk} H_{kn} \right] = 0, \quad j, n = 1, 2, \dots, N, \quad N \leq \infty \quad (13)$$

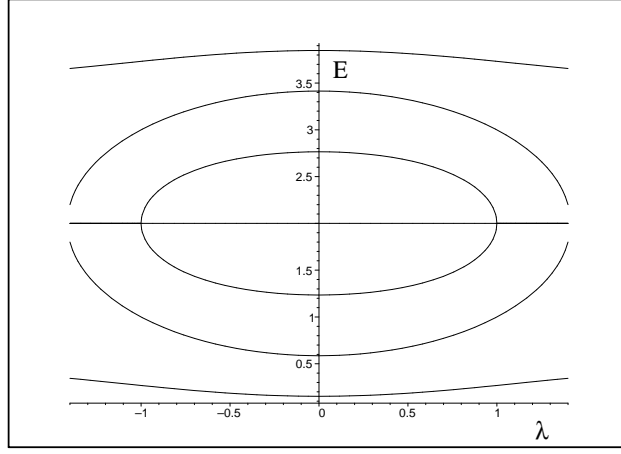


Figure 2: The λ -dependence of energies at $N = 7$.

which is imposed either upon the heavily non-unique positive definite ansatz

$$\Theta = \left(\Theta_{(M)}^{(N)} \right)^{(S)} = \sum_{k=1}^M \mu_k \Theta_{(k)}^{(N)} > 0 \quad (14)$$

containing the suitable sparse, $(2k-1)$ -diagonal components $\Theta_{(k)}^{(N)}$ and defining the physical Hilbert-space metrics at any $M \leq N$, or upon the indefinite though still invertible metric \mathcal{P} in Krein space \mathbf{K} ,

$$\Theta = \mathcal{P} = \left(\Theta_{(M)}^{(N)} \right)^{(Krein)} = \sum_{k=1}^M \nu_k \Theta_{(k)}^{(N)} \quad (15)$$

or upon the metric in the slightly more general auxiliary Pontryagin space $\tilde{\mathbf{K}}$,

$$\Theta = \mathcal{P} = \left(\Theta_{(M)}^{(N)} \right)^{(Pontryagin)} = \sum_{k=1}^M \rho_k \Theta_{(k)}^{(N)}. \quad (16)$$

In the case of the former Eq. (15) we shall assume that the respective numbers N_- and N_+ of the negative and positive eigenvalues of Θ will be roughly the same and, in any case, infinite in the limit $N \rightarrow \infty$. In the latter case of Eq. (16) one of the *non-equal* numbers N_- and N_+ should stay, by the definition of Pontryagin spaces, finite in the limit $N \rightarrow \infty$.

5 The Hilbert/Krein/Pontryagin classification of auxiliary spaces

For the sake of brevity of our present considerations we shall keep the dimension N finite and fixed and even. We shall speak about the “Krein-space-simulating case” if $N_- = N_+$ and about the “Pontryagin-space case” if $0 \neq N_- \neq N_+ \neq 0$.

5.1 The non-numerical diagonal solution of Dieudonné equation.

In Ref. [15] we may find the explicit and, up to an inessential overall factor, unique diagonal solution of Eq. (13),

$$\Theta^{(N)}(\lambda) = \left(\Theta_{(1)}^{(N)} \right)^{(S)} = \begin{bmatrix} \alpha & 0 & \dots & 0 & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & 0 \\ 0 & 0 & \dots & 0 & \alpha \end{bmatrix}$$

with

$$\alpha = \alpha(\lambda) = \frac{1 - \lambda}{1 + \lambda}.$$

Inside the open interval of $\lambda \in (-1, 1)$ the latter quantity remains positive so that just the Hilbert-space solution (14) is obtained at $M = 1$. In our present paper we may speak about the $N_- = 0$ case or about the signature denoted, at an illustrative $N = N_+ = 8$, by the symbol $\boxed{+++++++}$ which displays the set of the signs of the eigenvalues of Θ in question.

5.2 The bidiagonal, indefinite solutions of Dieudonné' equation

Obviously, in a search for the indefinite metrics in \mathbf{K} or $\tilde{\mathbf{K}}$ we must study metrics (15) or (16) with $M = 2$ at least. Firstly, recalling the results of Ref. [15] we find the bidiagonal solution of Eq. (13) (with $\nu_1 = 0$ and inessential ν_2 in Eq. (15)) which is very sparse and, up to the overall factor $\nu_2 > 0$, unique,

$$\Theta^{(N)}(\lambda) = \left(\Theta_{(2)}^{(N)} \right)^{(Krein)} = \begin{bmatrix} 0 & \beta & 0 & 0 & \dots & 0 \\ \beta & 0 & 1 & 0 & \dots & 0 \\ 0 & 1 & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & 0 & 1 & 0 \\ \vdots & \ddots & 0 & 1 & 0 & \beta \\ 0 & \dots & 0 & 0 & \beta & 0 \end{bmatrix}. \quad (17)$$

This matrix contains the single positive variable $\beta = \beta(\lambda) = 1 - \lambda$ and may be classified as a (slightly non-standard) Krein-space metric. Its non-standard status results from its non-involutivity property

$$\left[\left(\Theta_{(2)}^{(N)} \right)^{(Krein)} \right]^2 \neq I.$$

This implies that the involutive Krein-space metric \mathcal{P} must be constructed via the preliminary diagonalization of matrix (17), i.e., via the evaluation of the set of its eigenvalues and, if needed, eigenvectors. In an illustrative example, let us pick up $N = 8$. Then, at $\beta = 1$ the numerically evaluated

Table 1: The sample of the coupling-dependence of eigenvalues and of the signatures for the tridiagonal metrics Θ of Eq. (19) at $N = 8$.

λ	(doubly degenerate) eigenvalues of $\Theta^{(8)}(\lambda)$	signature	classification
-1	1.885199025, 1.103209260, 0.1798728781, -0.6682811631	$+++++--$ regular,	acceptable \mathcal{P} , Pontryagin space
-0.5	2.325566538, 1.335120809, 0.07897024957, -0.9396575972	$+++++--$ regular,	acceptable \mathcal{P} , Pontryagin space
0	2.53208889, 1.34729636, 0, -0.879385241	$++++00--$ singular,	exceptional, not acceptable
0.5	2.10869763, 0.981936410, 0.0376599205, -0.328293960	$+++++--$ regular,	acceptable \mathcal{P} , Pontryagin space
0.95	1.66131164, 0.785034968, 0.0809096799, -0.0016321045	$+++++--$ regular,	acceptable \mathcal{P} , Pontryagin space
1	1.62348980, 0.777479066, 0.099031132, 0	$+++++00$ singular,	exceptional, not acceptable
1.1	1.555271054, 0.7692404001, 0.1312085969, -0.003231363463	$+++++--$ regular,	off domain, Pontryagin space
2	1.235525737, 0.8538808152, 0.1508170150, -0.04022356696	$+++++--$ regular,	off domain, Pontryagin space
200	1.000040269, 0.9999844811, 0.00002499875, -0.000024748775	$+++++--$ close to singular,	far off domain, Pontryagin space
-200	1.000040631, 0.9999846191, 0.00002499875, -0.000025248725	$+++++--$ close to singular,	far off domain, Pontryagin space

sample of eigenvalues is ± 1.87938524 , ± 1.53208889 , ± 1 and ± 0.347296355 . In other words, the eight-dimensional matrix (17) may be assigned the Krein-space-representing signature (i.e., the set of the signs of the eigenvalues) $++++--$ as well as a certain “generalized-parity” status at $\beta = 1$.

A slightly uncomfortable shortcoming of the similar *constructive* definitions of the auxiliary space \mathbf{K} lies in the natural dimension- and Hamiltonian-dependence of the metrics $\Theta^{(N)}(\lambda)$. Fortunately, their signature is changing rarely. For example, at the same dimension $N = 8$ the transition to a very small quantity $\beta = 0.02$ still gives the spectrum ± 1.80196162 , ± 1.24709165 , ± 0.445529554 , ± 0.00039952 compatible with the same Krein-space signature $++++--$.

5.3 The more-diagonal indefinite solutions of Dieudonné equation

According to Ref. [15] the general more-than-two-diagonal and maximally sparse solution of the Dieudonné equation still has the unique form at all N ,

$$\Theta_{(k)}^{(N)}(\lambda) = \begin{bmatrix} \dots & 0 & 0 & z & 0 & 0 & \dots \\ \dots & 0 & v & 0 & v & 0 & \dots \\ \ddots & v & 0 & 1 & 0 & v & \ddots \\ \ddots & 0 & 1 & 0 & 1 & 0 & \ddots \\ \ddots & 1 & 0 & 1 & 0 & 1 & \ddots \\ \ddots & 0 & 1 & 0 & 1 & 0 & \ddots \\ \ddots & \ddots & \ddots & \vdots & \ddots & \ddots & \ddots \end{bmatrix}. \quad (18)$$

It is defined in terms of the two functions of coupling λ ,

$$z = \gamma(\lambda) = \frac{1 - \lambda}{1 + \lambda^2}, \quad v = \delta(\lambda) = \frac{1}{1 + \lambda^2}.$$

For illustrative purposes we selected just the simplest, tridiagonal special case,

$$\Theta_{(3)}^{(N)}(\lambda) = \begin{bmatrix} 0 & 0 & z & 0 & \dots & 0 \\ 0 & v & 0 & v & 0 & \dots & 0 \\ z & 0 & 1 & \ddots & \ddots & \ddots & \vdots \\ 0 & v & \ddots & \ddots & \ddots & v & 0 \\ \vdots & \ddots & \ddots & \ddots & 1 & 0 & z \\ 0 & \dots & 0 & v & 0 & v & 0 \\ 0 & & \dots & 0 & z & 0 & 0 \end{bmatrix} \quad (19)$$

and calculated, numerically, its eigenvalues and signatures at $N = 8$. The sample of results is displayed in Table 1. It shows that in our toy model there emerges the fully general but still sufficiently elementary and viable third, Pontryagin-space alternative to the most usual Hilbert-space signature $\boxed{+++++++}$ with $N_- N_+ = 0$ and to the PTSQM-related Krein-space signature $\boxed{++++-- --}$ with $N_- - N_+ = 0$. We have arrived at our conclusions.

Conjecture 5.1. *In place of the standard PTSQM strategy of choosing the sufficiently elementary Krein-space pseudometric \mathcal{P} of Eq. (4) in advance, it may prove more efficient to start from any given Hamiltonian with real spectrum and to construct the suitable PTSQM pseudometric \mathcal{P} as a diagonalized form of any sparse solution Θ of the Dieudonné's Eq. (13).*

Corollary 5.2. *Once a given Hamiltonian \hat{H} and a self-adjoint and a boundedly-invertible bounded operator Θ satisfy Eq. (13) with $N \leq \infty$, the latter operator may play the role of the metric either (i.e., if positive definite) in the standard Hilbert space $\mathbf{H}^{(S)}$ of states, or (i.e., if $N_- = N_+$) in the auxiliary PTSQM Krein space \mathbf{K} or, thirdly (i.e., if $N_- \neq N_+$), in an alternative auxiliary Pontryagin space $\tilde{\mathbf{K}}$.*

6 Summary

Within the present extended version of \mathcal{PT} -symmetric quantum mechanics we still start working with Hamiltonians \hat{H} defined in an auxiliary, first, *unphysical* Hilbert space $\mathbf{H}^{(F)}$ where $\hat{H} \neq \hat{H}^\dagger$ is allowed non-Hermitian. In an intermediate step we propose to replace $\mathbf{H}^{(F)}$ *either* by Krein space \mathbf{K} *or* by Pontryagin space $\tilde{\mathbf{K}}$. Secondly, in place of the traditional selection of the (indefinite) metric $\mathcal{P} = \mathcal{P}^\dagger$ *in advance* (i.e., typically, in the form of an operator of parity) we propose to proceed *constructively*. This means that we only assume that the Hamiltonian is self-adjoint in \mathbf{K} or $\tilde{\mathbf{K}}$, i.e., that it satisfies the Dieudonné equation $\hat{H}^\dagger \mathcal{P} = \mathcal{P} \hat{H}$ where the operator (or matrix) \mathcal{P} is *not* given in advance and must be constructed and/or chosen out of a broader menu.

It has been multiply tested in the past that with many pre-selected unphysical Hilbert spaces $\mathbf{H}^{(F)}$ and Krein-space metrics \mathcal{P} the validity of the Dieudonné's equation opened the way towards the necessary and ultimate transition to the “second”, *physical* Hilbert space $\mathbf{H}^{(S)}$. In our present paper we tested and verified the feasibility of the similar transition $\mathbf{H}^{(F)} \rightarrow \mathbf{H}^{(S)}$ under the assumption that the auxiliary indefinite metric (or, if you wish, the pseudometric) \mathcal{P} only specifies the less usual, Pontryagin intermediate space $\tilde{\mathbf{K}}$.

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